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An evaluation of amplitude occurring in ionization of H by $e^{\pm}$ impact

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Abstract : An efficient evaluation of the amplitude of ionization of hydrogen atom by $e^{\pm}$ impact is presented without any ambiguity. The final state is represented by the product of three Coulomb functions satisfying the correct asymptotic condition. Results are reported for the double differential cross section at forward ejection angle as a function of ejection energy and compared with the available theoretical findings.

Keywords : Ionization amplitude, double differential cross section, asymptotic form, hypergeometric function.

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We consider in this communication the evaluation of the amplitude occurring in ionization of atomic hydrogen under electron or positron impact using the product of three confluent hypergeometric functions (${}_1F_1$) for the final state wave function as given by Brauner *et al* [1] which has the correct asymptotic form. As we shall see later, the ionization amplitude is obtained after a double integration of an integral which is a multiple valued function. To determine the correct value of this integrand is of vital importance, if one uses the incorrect branch, one gets entirely wrong results and faces abrupt discontinuity. The derivation of the general expression leading to the correct value of this multi-valued integrand is the main contribution of the present work.

We now consider the six dimensional mother integral involving three ${}_1F_1$ functions, from which the ionization amplitude is derivable by parametric differentiation [2]

$$
\begin{aligned}
I &= N \int e^{iq_m \cdot r_1 - ik_2 r_2} \times e^{-\lambda_1 r_2} \times \frac{1}{r_1 r_2 r_{12}} \\
&\times {}_1F_1\{i\alpha_1 \cdot 1, i(k_1 r_1 + k_1 \cdot r_1)\} \\
&\times {}_1F_1\{i\alpha_2, 1, i(k_2 r_2 + k_2 \cdot r_2)\} \times {}_1F_1\{i\alpha_3, 1, i(q r_{12} + q \cdot r_{12})\} \\
&\times dr_1 dr_2, \qquad (1)
\end{aligned}
$$

where $q_m = k_i - k_1$ and k_i, k_1, k_2 are the momenta of the incident and scattered positron (electron) and the ejected electron respectively. r_1 and r_2 are the position vectors of positron (electron) and electron. Further,

$$
\alpha_1 = -\frac{Z_P Z_T}{k_1}, \quad \alpha_2 = \frac{Z_T}{k_2} \text{ and } \alpha_3 = \frac{Z_P}{|k_1 - k_2|},
$$

$$
q = (1/2)(k_1 - k_2) \quad \text{and } r_{12} = r_1 - r_2. \qquad (2)
$$

Z_P and Z_T being the projectile and target charges respectively; N being a constant. Our method of integration of integral in eq. (1) is modelled after the elegant work of Nordsieck [3], who first evaluated by contour integration method the matrix element integrals for bremsstrahlung and pair production involving two ${}_1F_1$ functions in terms of appropriate Gauss hypergeometric functions with a real argument lying between 0 and 1. He represented the special hypergeometric function by the following closed contour integral

$$
F_1(i\alpha, 1, Z) = \frac{1}{2\pi i} \oint^{(0+,\,1+)} p(\alpha, t)\, e^{Zt}\, dt,
$$

where $\quad p(\alpha, t) = t^{i\alpha - 1} (t-1)^{-i\alpha} \qquad (3)$

There is a branch cut from 0 to 1 and the phases of t and $(t - 1)$ are fixed by taking both of them as zero at the point where the contour crosses the real axis to the right of 1. The phase of each variable which is measured from the positive real axis is positive when counter clock wise and negative when clockwise and cannot exceed the value π. Using Nordsieck representation (eq. (3)) for the three ${}_1F_1$ functions in eq. (1) with t_1, t_2 and t_3 as integration variables, we get

$$
I = \frac{N}{(2\pi i)^3} \int dt_1\, dt_2\, dt_3\, p(\alpha_1, t_1)\, p(\alpha_2, t_2)\, p(\alpha_3, t_3)\, J, \qquad (4)
$$

where

$$
\begin{aligned}
J = \underset{\substack{\mu \to 0^+ \\ \eta \to 0^+}}{Lt} &\int dr_1\, dr_2 \frac{1}{r_1 r_2 r_{12}} e^{-\eta_1 r_1 - \mu_1 r_{12} - \lambda_1 r_2} e^{i(q_m + t_1 k_1) \cdot r_1} \\
&e^{-i(k_2 - t_2 k_2) r_2} \times e^{i t_3 q r_{12}}, \qquad (5)
\end{aligned}
$$

with $$\lambda_1 = \lambda_t - it_2k_2, \quad \mu_1 = \mu - it_3q, \quad \eta_1 = \eta - it_1k_1. \tag{6}$$

We carry out first, the space integration to get a Lewis integral function [4]. For the convenience of later integration with respect to t_1 and t_2, we express, following Sinha and Sil [5], the Lewis function as

$$J = 16\pi^2 \int \frac{dv}{\alpha v^2 + 2\beta v + \gamma}, \tag{7}$$

where α, β, γ are linear functions of t_1 or t_2. Thus we can write $(\alpha v^2 + 2\beta v + \gamma)$ as $(A + Bt_1 + Ct_2 + Dt_1t_2)$ where A, B, C, D are functions of t_3 and v, in addition to other constant parameters. Hence, eq. (7) can be recast into the form

$$J = 16\pi^2 \int \frac{dv}{A + Bt_1 + Ct_2 + Dt_1t_2}. \tag{8}$$

Putting the expression (8) for J in eq. (4) we have

$$I = \frac{16\pi^2 N}{(2\pi i)^3} \oint \int_0^\infty \frac{dt_1\, dt_2\, dt_3\, p(\alpha_1, t_1)\, p(\alpha_2, t_2)\, p(\alpha_3, t_3) dv}{A + Bt_1 + Ct_2 + Dt_1t_2}. \tag{9}$$

Eq. (9) can be written as

$$I = \frac{16\pi^2 N}{2\pi i} \oint dt_3\, p(\alpha_3, t_3) \int^\infty dv\, I_c, \tag{9a}$$

where

$$I_c = \frac{1}{(2\pi i)^2} \times \frac{1}{A} \oint\oint \frac{dt_1\, dt_2\, p(\alpha_1, t_1)\, p(\alpha_2, t_2)}{1 + Xt_1 + Yt_2 + Zt_1t_2}, \tag{10}$$

and $$X = \frac{B}{A}, \quad Y = \frac{C}{A} \quad \text{and} \quad Z = \frac{D}{A}.$$

For the evaluation of the above integral, we write down it into the following form

$$I_c = \frac{}{(2\pi i)^2} \times \frac{1}{A} \int\int_{\Gamma_1 \Gamma_2} \frac{dt_1\, dt_2\, p(\alpha_1, t_1)\, p(\alpha_2, t_2)}{(1 + Xt_1)(1 + Yt_2)\left[1 + \frac{t_1t_2\Delta}{(1 + Xt_1)(1 + Yt_2)}\right]} \tag{11}$$

with $\Delta = Z - XY$.

Let us first assume $\frac{\Delta}{(1+Xt_1)(1+Yt_2)}$ to be very small and carry out the evaluation of the integral. Later, this restriction will be removed by analytic continuation. We expand $\left[1+\frac{t_1t_2\Delta}{(1+Xt_1)(1+Yt_2)}\right]^{-1}$ and express

$$I_r = \frac{1}{(2\pi i)^2} \times \frac{1}{A}\sum_{r=0}\int_{\Gamma_1}\int_{\Gamma_2} dt_1\, dt_2\, p(\alpha_1, t_1)\, p(\alpha_2, t_2)$$

$$\frac{(-1)^r \Delta^r t_1^r t_2^r}{(1+Xt_1)^{r+1}(1+Yt_2)^{r+1}}. \tag{12}$$

Eq. (12) is separable in t_1 and t_2 and each term of the series can be integrated by residue calculation.

Now let us consider the evaluation of the general term

$$\int_{\Gamma}^{(0+,1+)} \frac{dt\, t^{-1+i\alpha}(t-1)^{-i\alpha}\, t^r}{(1+Xt)^{r+1}}, \tag{13}$$

which has a multiple pole of $(r+1)$-th order at '$-\frac{1}{X}$'.

We note that on the infinite circle $|t| \to \infty$, the integrand is single valued and $O\left(\frac{1}{|t|^2}\right)$ and hence the integral over the infinite circle vanishes. Since the pole at '$-\frac{1}{X}$' is outside the contour Γ,

We have

$$\int \frac{p(\alpha,t)dt}{(1+Xt)} + 2\pi i\frac{p\left(\alpha, -\frac{1}{X}\right)}{X}$$

= integral over the infinite circle = 0

whence

$$\int \frac{p(\alpha,t)dt}{(1+Xt)} = -2\pi i\, p\left(\alpha, -\frac{1}{X}\right)\Big/X = 2\pi i(1+X)$$

By r-th order differentiation we get

$$\int_{\Gamma}^{(0+,1+)} \frac{dt\, t^{r-1+i\alpha}(t-1)^{-i\alpha}}{(1+Xt)^{r+1}} = 2\pi i\frac{(i\alpha)_r}{r!}(1+X)^{-} \tag{14}$$

using Pochhamer symbols

$$(i\alpha)_r = i\alpha(i\alpha+1).....(i\alpha+r-1) \text{ and } (i\alpha)_0 = 1.$$

Hence, we can write

$$I_c = \frac{1}{A} \times \frac{1}{(1+X)_1^{i\alpha}\ 1(1+Y)_2^{i\alpha}} \sum_{r=0}^{\infty} \frac{(i\alpha_1)_r\ (i\alpha_2)_r}{r!\ (1)_r}$$

$$\times \left\{- \frac{\Delta}{(1+X)\ (1+Y)}\right\}^r. \tag{15}$$

The above series when convergent can easily be identified as the representation of ${}_2F_1(i\alpha_1, i\alpha_2, 1, Z)$ for $|Z| < 1$, so, we have

$$I_c = \frac{1}{A}(1+X)^{-i\alpha_1}(1+Y)^{-i\alpha_2}\ {}_2F_1\left(i\alpha_1, i\alpha_2, 1, Z\right) \tag{16}$$

where $$Z = -\frac{\Delta}{(1+X)\ (1+Y)} = \frac{BC-AD}{(A+B)\ (A+C)}.$$

Thus, we can write

$$I_c = \frac{1}{A}\left(\frac{A}{A+B}\right)^{i\alpha_1}\left(\frac{A}{A+C}\right)^{i\alpha_2}\ {}_2F_1\left(i\alpha_1, i\alpha_2, 1, Z\right). \tag{17}$$

The value of this multiple valued function can be computed correctly without any ambiguity following the phase convention of Nordsieck [3]. The result which is obtained for $|Z| < 1$, can be extended for any arbitrary value of Z by analytic continuation.

In the method of Nordsieck [3], the result of the first 't_1' integration was carried out by residue calculation as we have followed. He then recast the integrand to an appropriate form, so that, after transformation of the integration variable and changing over to suitable contour, the final result was obtained in terms a Gauss hypergeometric function, the argument 'Z' of which is real positive and < 1, so that ordinary series representation could be used for its evaluation. This 't_2' integration required an elaborate and careful analysis by Nordsieck, of the physically possible values of the parameters of the problems considered by him *viz.*, bremsstrahlung and pair-production. In our case it is not possible to obtain adequate information of the relevant parameters. But we are able to give a simple derivation of a general expression which yields the correct result for the integral without requiring any such information. It should be noted that the result obtained by Nordsieck are different in form but each result for his two problems is the appropriate analytic continuation of our general expression for the relevant physical parameters of the problem.

Incidentally, it may be pointed out that the representation of the functions ${}_1F_1(i\alpha, 1, Z)$ and ${}_2F_1(a, b, c, Z)$ as given by Brauner *et al* in their work [1] [eq. (A18), (A19) and (A24)] is not beyond objection mathematically, since the real part of 'a' of ${}_1F_1(a, c, z)$ is zero and the condition given by Erdelyi' *et al* [6] is not satisfied, similar is the case with the ${}_2F_1(a, b, c, z)$ in eq. (A24) of Brauner *et al* [1].

The justification of these representations needs a convergence factor 'ε' to be put 'zero' ultimately. Moreover, there is no guide line to follow for the computation of the correct and unambiguous value of the multiple valued function.

We present here the double differential cross section results (DDCS) integrated over the scattering angles for the ionization of hydrogen atom by positron impact. The DDCS can be expressed as (atomic units) :

$$\frac{d^2\sigma}{dE_2 d\Omega_2} = \frac{16\pi^4 k_1 k_2}{k_i} \int \left|T_{fi}\right|^2 d\Omega_1 \tag{18}$$

where
$$T_{fi} = \underset{\substack{\mu\to 0\\ \eta\to 0}}{Lt} \left(\frac{\partial^2 I}{\partial\lambda_1 \partial\mu_1} - \frac{\partial^2 I}{\partial\lambda_1 \partial\eta_1} \right). \tag{19}$$

To find out the value of T_{fi}, we have to carry out the t_3 and v integrations occurring in I (eq. 9(a)). Following the procedure adopted by Roy *et al* [7], we have performed the t_3 and v integrations numerically. Before numerical integrations, all the parametric differentiations and limiting values in eq. (19) are to be considered.

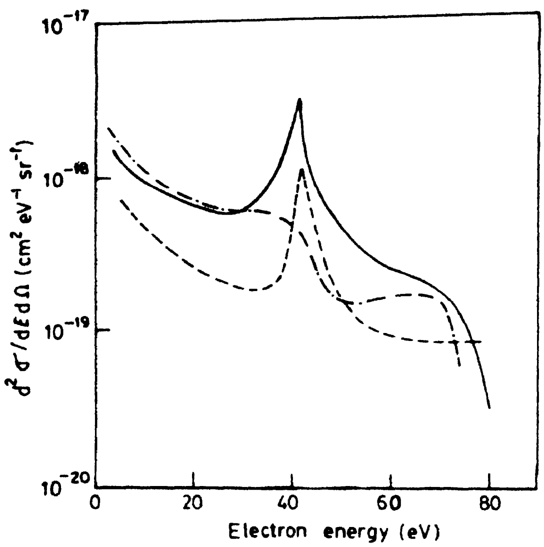

Figure 1. The double differential ionization cross section for the impact of positron on atomic hydrogen as a function of the electron ejection energy for 0° ejection angle.
Present result (—); result of Mandal *et al* (- - -); result of Schultz and Reinhold (—● —● —●) for $\theta_2 = 2°$.

Further, we may mention that the Gauss hypergeometric functions (${}_2F_1$) occurring in eq. (17) contains in general a complex argument. A general method for the evaluation of the function over the entire complex plane has been developed and described in details by Roy *et al* [8] who have made use of different series representations of the function to ensure its quick, efficient and accurate evaluation. We follow their method for the evaluation of $_2F_1$ most efficiently.

In Figure 1, we display our DDCS values at forward ejection angle for the incident energy 100 eV as a function of ejection energies. Here we compare our results with those of Mandal *et al* [9] for $\theta_2 = 0°$ and also with the values of Schultz and Reinhold [10] for $\theta_2 = 2°$. In our calculation, we find that the DDCS values are almost identical for $\theta_2 = 0°$ and 2°. The results of Mandal *et al* using the three body scattering formalism of Faddeev [11] are much lower than our values. The results obtained by Schultz and Reinhold with the help of Classical Trajectory Monte Carlo technique are in good agreement with our results at lower and higher ejection energies. Further, our curve shows the presence of a cusp in conformity with the findings of Mandal *et al* and a ridge like structure at higher ejection energies found in the curve of Schultz and Reinhold.

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*[An Erratum of this work has been submitted to Phys. Rev. A in which numerical values of DDCS curve has decreased though the structure remained the same]